

Author index to volume 145

Aguilar, A., B. Brunetti, M. González and F. Vecchiocattivi, A crossed beam study of the ionization of molecules by metastable neon atoms	145 (1990) 211
Alexander, M.H., see B. Pouilly	145 (1990) 191
Allen, W.D., Y. Yamaguchi, A.G. Császár, D.A. Clabo Jr., R.B. Remington and H.F. Schaefer III, A systematic study of molecular vibrational anharmonicity and vibration-rotation interaction by self-consistent-field higher-derivative methods. Linear polyatomic molecules	145 (1990) 427
Angstl, R., Calculation of molecular <i>g</i> tensors. Comparison of Rayleigh-Schrödinger and Hartree-Fock perturbation theory	145 (1990) 413
Aquilanti, V., R. Candori, D. Cappelletti, E. Luzzatti and F. Pirani, Scattering of magnetically analyzed F(² P) atoms and their interactions with He, Ne, H ₂ and CH ₄	145 (1990) 293
Aspect, A., N. Vansteenkiste, R. Kaiser, H. Haberland and M. Karrais, Preparation of a pure intense beam of metastable helium by laser cooling	145 (1990) 307
Bagryanskaya, E.G., see I.V. Koptyug	145 (1990) 375
Bancroft, G.M., see J.D. Bozek	145 (1990) 131
Baudon, J., F. Perales, Ch. Miniatura, J. Robert, G. Vassilev, J. Reinhardt and H. Haberland, Polarization effects in metastable neon atom (Ne*(³ P ₂)) on ground state neon atom collision at thermal energy	145 (1990) 153
Beijerinck, H.C.W., see E.J.D. Vredenbregt	145 (1990) 267
Bencivenni, L., see F. Ramondo	145 (1990) 27
Boom, W., see E.J.D. Vredenbregt	145 (1990) 267
Bozek, J.D., G.M. Bancroft and K.H. Tan, Resonances in the silicon L core level cross sections of fluoromethylsilane compounds characterized by photoabsorption spectroscopy and MS-X α calculations	145 (1990) 131
Braghetti, M., see H.A. Kołodziej	145 (1990) 355
Brion, C.E., see G. Cooper	145 (1990) 117
Brunetti, B., see A. Aguilar	145 (1990) 211
Caia, V., see H.A. Kołodziej	145 (1990) 355
Caminiti, R., see F. Ramondo	145 (1990) 27
Candori, R., see V. Aquilanti	145 (1990) 293
Cappelletti, D., see V. Aquilanti	145 (1990) 293
Castex, M.C., see F. Spiegelmann	145 (1990) 173
Chiu, Y.-N. and M. Gong, Spin symmetry and interaction mechanisms in free radical reactions	145 (1990) 397
Clabo Jr., D.A., see W.D. Allen	145 (1990) 427
Cooper, G., W. Zhang, C.E. Brion and K.H. Tan, Photoelectron spectroscopy of the freon molecules CF ₃ Cl, CF ₂ Cl ₂ and CFCl ₃ using synchrotron radiation from 41 to 160 eV	145 (1990) 117
Császár, A.G., see W.D. Allen	145 (1990) 427

Das, F.K., see S. Ramasesha	145 (1990) 343
Delaval, J.M., see J. Schamps	145 (1990) 101
Delos, J.B., see S.E. Haywood	145 (1990) 253
Distefano, G., see A. Modelli	145 (1990) 89
Dubicki, L., see M.J. Riley	145 (1990) 363
Faucher, O., see J. Schamps	145 (1990) 101
Friend, D.G., see C.A. Nieto de Castro	145 (1990) 19
Fünfschilling, J., see P. Petelenz	145 (1990) 333
Gadea, F.X., see F. Spiegelmann	145 (1990) 173
Getino, C., B.G. Sumpter and J. Santamaria, Intramolecular and reactive dynamics of OH-overtone excited HOOH(D): a classical trajectory study on a quasiseparable potential surface	145 (1990) 1
	145 (1990) 355
Głowiak, T., see H.A. Kołodziej	145 (1990) 397
Gong, M., see Y.-N. Chiu	145 (1990) 211
González, M., see A. Aguilar	145 (1990) 27
Grandinetti, F., see F. Ramondo	145 (1990) 375
Grishin, Yu.A., see I.V. Koptyug	145 (1990) 89
Guerra, M., see A. Modelli	
Gunde, R., T.-K. Ha and H.H. Günthard, Consistent force field modeling of matrix isolated molecules. V. Minimum energy path potential to the conformer conversion of 1,2-difluoroethane: Ar ₃₆₄ , ab initio calculation of electric multipole moments and electric polarization contribution to the conversion barrier	145 (1990) 37
Günthard, H.H., see R. Gunde	145 (1990) 37
Ha, T.-K., see R. Gunde	145 (1990) 37
Haberland, H., see J. Baudon	145 (1990) 153
Haberland, H., see A. Aspect	145 (1990) 307
Haywood, S.E. and J.B. Delos, A close-coupling theory of associative detachment of electrons from negative ions	145 (1990) 253
Hennecart, D., see H. Kucal	145 (1990) 163
Hotop, H., see A. Merz	145 (1990) 219
Jones, D., see A. Modelli	145 (1990) 89
Kaiser, R., see A. Aspect	145 (1990) 307
Karrais, M., see A. Aspect	145 (1990) 307
Kołodziej, H.A., T. Głowiak, S. Sorriso, V. Caia and M. Braghetti, The reorientational motion of substituted benzenes in the crystalline state. Dielectric relaxation of orthodinitrotetramethylbenzene and orthodinitrotetrachlorobenzene	145 (1990) 355
Koptyug, I.V., E.G. Bagryanskaya, Yu.A. Grishin and R.Z. Sagdeev, The main regularities of SNP formation in biradicals on the photolysis of cycloalkanones	145 (1990) 375
Krausz, E.R., see M.J. Riley	145 (1990) 363
Kucal, H., D. Hennecart and F. Masnou-Seeuws, Model potential methods for the treatment of collisions between an excited rare gas and a ground state rare gas: accuracy and limitations	145 (1990) 163

Ladik, J., see C.-M. Liegener 145 (1990) 385

Lermé, J., Iterative methods to compute one- and two-dimensional Franck-Condon factors. Tests of accuracy and application to study indirect molecular transitions 145 (1990) 67

Liegener, C.-M., A. Sutjianto and J. Ladik, The treatment of electron correlation in aperiodic systems. III. Application to polypeptides 145 (1990) 385

Luzzatti, E., see V. Aquilanti 145 (1990) 293

Malinovsky, A.L. and E.A. Ryabov, Intramolecular vibrational distribution in IR multi-photon excited $\text{CF}_3\text{CH}_2\text{OH}$ 145 (1990) 389

Masnou-Seeuws, F., see H. Kucal 145 (1990) 163

Merz, A., M.W. Müller, M.-W. Ruf, H. Hotop, W. Meyer and M. Movre, Experimental and theoretical studies of simple attractive Penning ionization systems 145 (1990) 219

Metcalf, H., see B. Sheehy 145 (1990) 317

Meyer, W., see A. Merz 145 (1990) 219

Miniatura, Ch., see J. Baudon 145 (1990) 153

Modelli, A., F. Scagnolari, G. Distefano, M. Guerra and D. Jones, Electronic structure of tert-butyl halides and group 14 derivatives: electron affinities and dissociative electron attachment 145 (1990) 89

Moran, G., see M.J. Riley 145 (1990) 363

Morgner, H., The validity of the local approximation in Penning ionization as studied by model calculations 145 (1990) 239

Movre, M., see A. Merz 145 (1990) 219

Müller, M.W., see A. Merz 145 (1990) 219

Nieto de Castro, C.A., D.G. Friend, R.A. Perkins and J.C. Rainwater, Thermal conductivity of a moderately dense gas 145 (1990) 19

Perales, F., see J. Baudon 145 (1990) 153

Perkins, R.A., see C.A. Nieto de Castro 145 (1990) 19

Petelenz, P. and J. Fünfschilling, Resonantly enhanced external heavy atom effect in organic glasses 145 (1990) 333

Pirani, F., see V. Aquilanti 145 (1990) 293

Pouilly, B. and M.H. Alexander, A new look at the retention of orbital alignment in collisions involving atoms in ${}^1\text{P}$ electronic states: $\text{Ca}(4s5p\,{}^1\text{P}) + \text{He}$ 145 (1990) 191

Rainwater, J.C., see C.A. Nieto de Castro 145 (1990) 19

Ramasesha, S. and P.K. Das, Second harmonic generation coefficients in push-pull polyenes: a model exact study 145 (1990) 343

Ramondo, F., L. Bencivenni, R. Caminiti and F. Grandinetti, Coordination structures and vibrational frequencies of Li and Na metaphosphates and nitrates. An ab initio SCF study 145 (1990) 27

Reinhardt, J., see J. Baudon 145 (1990) 153

Remington, R.B., see W.D. Allen 145 (1990) 427

Riley, M.J., L. Dubicki, G. Moran, E.R. Krausz and I. Yamada, Absorption and magnetic circular dichroism spectra of the compressed copper(II) ion in K_2ZnF_4 145 (1990) 363

Robert, J., see J. Baudon 145 (1990) 153

Ruf, M.-W., see A. Merz 145 (1990) 219

Ryabov, E.A., see A.L. Malinovsky 145 (1990) 389

Sagdeev, R.Z., see I.V. Koptyug	145 (1990) 375
Santamaria, J., see C. Getino	145 (1990) 1
Scagnolari, F., see A. Modelli	145 (1990) 89
Schaefer III, H.F., see W.D. Allen	145 (1990) 427
Schamps, J., J.M. Delaval and O. Faucher, A calculation of radiative lifetimes of electronically excited rovibronic levels of CuF	145 (1990) 101
Shang, S.-Q., see B. Sheehy	145 (1990) 317
Sheehy, B., S.-Q. Shang, P. van der Straten and H. Metcalf, Collimation of a rubidium beam below the Doppler limit	145 (1990) 317
Shimizu, F., K. Shimizu and H. Takuma, A high intensity metastable neon trap	145 (1990) 327
Shimizu, K., see F. Shimizu	145 (1990) 327
Song, G., Non-empirical calculation of the Whitten-Rabinovitch coefficient	145 (1990) 111
Sorriso, S., see H.A. Kołodziej	145 (1990) 355
Spiegelmann, F., F.X. Gadea and M.C. Castex, Theoretical study of the electronic structure of the ArKr* exciplex	145 (1990) 173
Sumpter, B.G., see C. Getino	145 (1990) 1
Sutjianto, A., see C.-M. Liegener	145 (1990) 385
Takuma, H., see F. Shimizu	145 (1990) 327
Tan, K.H., see G. Cooper	145 (1990) 117
Tan, K.H., see J.D. Bozek	145 (1990) 131
Van der Straten, P., see B. Sheehy	145 (1990) 317
Van Gerwen, R.J.F., see E.J.D. Vredenbregt	145 (1990) 267
Vansteenkiste, N., see A. Aspect	145 (1990) 307
Vassilev, G., see J. Baudon	145 (1990) 153
Vecchiocattivi, F., see A. Aguilar	145 (1990) 211
Vredenbregt, E.J.D., W. Boom, R.J.F. van Gerwen and H.C.W. Beijerinck, Excitation transfer collisions of metastable Ar*, Kr* and Xe* atoms with N ₂ (X, ν=0): collision energy dependence of excitation cross sections and product vibrational distribution of N ₂ (C ³ Π _u , ν'=0,1,2,3)	145 (1990) 267
Yamada, I., see M.J. Riley	145 (1990) 363
Yamaguchi, Y., see W.D. Allen	145 (1990) 427
Zhang, W., see G. Cooper	145 (1990) 117

List of subjects

1 METHODS

1.1 Theoretical

- 1.1.1 Group theory and algebras *
- 1.1.2 Classical mechanics *
- 1.1.3 Quantized field theory
- 1.1.4 Many body and quasiparticle approaches *
- 1.1.5 Coupling schemes and perturbative treatments *
- 1.1.6 Relativistic quantum mechanics *
- 1.1.7 Transport quantum mechanics
- 1.1.8 Equilibrium statistical mechanics
- 1.1.9 Statistical mechanics of stationary states
- 1.1.10 Non-equilibrium thermodynamic and hydrodynamic theories *
- 1.1.11 Ab initio schemes for stationary properties *
- 1.1.12 Computational and simulation methods *
- 1.1.13 Molecular dynamics and scattering theory *

1.2 Experimental

- 1.2.1 Magnetic resonances *
- 1.2.2 Cyclotron resonance
- 1.2.3 Microwave spectroscopy *
- 1.2.4 Infrared spectroscopy
- 1.2.5 Raman spectroscopy *
- 1.2.6 Visible and UV spectroscopy *
- 1.2.7 Fluorescence spectroscopy
- 1.2.8 Photoelectron and Auger spectroscopy *
- 1.2.9 X-ray spectroscopy *
- 1.2.10 Electron impact spectroscopy *
- 1.2.11 Laser methods *
- 1.2.12 Picosecond spectroscopy
- 1.2.13 Non-linear optical spectroscopy
- 1.2.14 Synchrotron spectroscopies *
- 1.2.15 Coherent optical spectroscopy *
- 1.2.16 Optical pumping *
- 1.2.17 Multiple resonance spectroscopy *
- 1.2.18 Optoacoustic spectroscopy
- 1.2.19 Atomic and molecular beam techniques *
- 1.2.20 Time-resolved experiments *
- 1.2.21 Mass spectrometry
- 1.2.22 Radiolysis
- 1.2.23 Mössbauer spectroscopy
- 1.2.24 X-ray, electron and neutron diffraction
- 1.2.25 Neutron scattering
- 1.2.26 Light scattering
- 1.2.27 Field emission and field ionization
- 1.2.28 Measurement of macroscopic variables *

2 OBJECTS

2.1 Bulk systems

- 2.1.1 Gases *
- 2.1.2 Supersonic beams *
- 2.1.3 Liquids neat
- 2.1.4 Liquid mixtures and solutions *
- 2.1.5 Crystals *
 - 2.1.5.1 neat
 - 2.1.5.2 mixed *
- 2.1.6 Glasses *
- 2.1.7 Liquid crystals
- 2.1.8 Polymers *
- 2.1.9 Semiconductors
- 2.1.10 Metals and alloys
- 2.1.11 Thin films
- 2.1.12 Surfaces
- 2.1.13 Low-dimensional materials
- 2.1.14 Dielectrics
- 2.1.15 Plasmas *
- 2.1.16 Biological systems

2.2 Microscopic systems

- 2.2.1 Atoms *
- 2.2.2 Molecules (neutral and ionic) *
 - 2.2.2.1 diatomic *
 - 2.2.2.2 small polyatomics *
 - 2.2.2.3 aromatics *
 - 2.2.2.4 other large
- 2.2.2.5 polymeric and biological *
- 2.2.3 Molecular aggregates *
 - 2.2.3.1 dimers
 - 2.2.3.2 van der Waals molecules *
 - 2.2.3.3 clusters *
 - 2.2.3.4 complexes
- 2.2.4 Free radicals (including hydronium and muonium) *
- 2.2.5 Quasiparticles (including excitons)
- 2.2.6 Defects and impurities
- 2.2.7 Ions and charge carriers *

* Denotes subjects covered in this volume

3 PHENOMENA

3.1	Molecular structure *	3.16	Multiphoton phenomena *
3.2	Vibrations and rotations of molecules *	3.17	Reactions (including dissociation) *
3.3	Electronic structure and states *	3.17.1	gas phase *
3.4	Electric and magnetic properties *	3.17.2	condensed phase
3.5	Spin splittings	3.17.3	photochemical *
3.6	Optical activity	3.18	Tunnelling
3.7	Molecular interactions *	3.19	Electron transfer
3.8	Spectral bandshapes and intensities *	3.20	Positron annihilation
3.9	Coupling of electronic and nuclear motion *	3.21	Ionization (including Rydberg states) *
3.10	Energy transfer processes *	3.22	Molecular motion (including diffusive) *
3.11	Molecular photophysical processes *	3.23	Isotopic effects
3.12	Intramolecular dynamics *	3.24	Fluctuations and noise
3.12.1	radiationless transitions	3.25	Collective motion and excitations
3.12.2	vibrational energy redistribution (including vibrational dissociation) *	3.26	Surface effects and catalysis
3.13	Luminescence spectra, yields and lifetimes *	3.27	Thermodynamic and transport properties *
3.14	Coherence loss processes	3.28	Structure of solids and liquids
3.15	Non-linear responses (including optical)	3.29	Critical phenomena
		3.30	Phase transitions *

Subject index to volume 145

METHODS

Theoretical

Group theory and algebras

Spin symmetry and interaction mechanisms in free radical reactions, Y.-N. Chiu and M. Gong

145 (1990) 397

Classical mechanics

Intramolecular and reactive dynamics of OH-overtone excited HOOH(D): a classical trajectory study on a quasiseparable potential surface, C. Getino, B.G. Sumpter and J. Santamaria

145 (1990) 1

Many body and quasiparticle approaches

The treatment of electron correlation in aperiodic systems. III. Application to polypeptides, C.-M. Liegener, A. Sutjianto and J. Ladik

145 (1990) 385

Coupling schemes and perturbative treatments

Theoretical study of the electronic structure of the ArKr* exciplex, F. Spiegelmann, F.X. Gadea and M.C. Castex

145 (1990) 173

The validity of the local approximation in Penning ionization as studied by model calculations, H. Morgner

145 (1990) 239

A close-coupling theory of associative detachment of electrons from negative ions, S.E. Haywood and J.B. Delos

145 (1990) 253

Calculation of molecular *g* tensors. Comparison of Rayleigh–Schrödinger and Hartree–Fock perturbation theory, R. Angstl

145 (1990) 413

Relativistic quantum mechanics

Theoretical study of the electronic structure of the ArKr* exciplex, F. Spiegelmann, F.X. Gadea and M.C. Castex

145 (1990) 173

Non-equilibrium thermodynamic and hydrodynamic theories

Thermal conductivity of a moderately dense gas, C.A. Nieto de Castro, D.G. Friend, R.A. Perkins and J.C. Rainwater

145 (1990) 19

Ab initio schemes for stationary properties

Coordination structures and vibrational frequencies of Li and Na metaphosphates and nitrates. An ab initio SCF study, F. Ramondo, L. Bencivenni, R. Caminiti and F. Grandinetti

145 (1990) 27

Consistent force field modeling of matrix isolated molecules. V. Minimum energy path potential to the conformer conversion of 1,2-difluoroethane: Ar₃₆₄, ab initio calculation of electric multipole moments and electric polarization contribution to the conversion barrier, R. Gunde, T.-K. Ha and H.H. Günthard 145 (1990) 37

Theoretical study of the electronic structure of the ArKr* exciplex, F. Spiegelmann, F.X. Gadea and M.C. Castex 145 (1990) 173

Experimental and theoretical studies of simple attractive Penning ionization systems, A. Merz, M.W. Müller, M.-W. Ruf, H. Hotop, W. Meyer and M. Movre 145 (1990) 219

A systematic study of molecular vibrational anharmonicity and vibration-rotation interaction by self-consistent-field higher-derivative methods. Linear polyatomic molecules, W.D. Allen, Y. Yamaguchi, A.G. Császár, D.A. Clabo Jr., R.B. Remington and H.F. Schaefer III 145 (1990) 427

Computational and simulation methods

Intramolecular and reactive dynamics of OH-overtone excited HOOH(D): a classical trajectory study on a quasiseparable potential surface, C. Getino, B.G. Sumpter and J. Santamaría 145 (1990) 1

Consistent force field modeling of matrix isolated molecules. V. Minimum energy path potential to the conformer conversion of 1,2-difluoroethane: Ar₃₆₄, ab initio calculation of electric multipole moments and electric polarization contribution to the conversion barrier, R. Gunde, T.-K. Ha and H.H. Günthard 145 (1990) 37

Iterative methods to compute one- and two-dimensional Franck-Condon factors. Tests of accuracy and application to study indirect molecular transitions, J. Lermé 145 (1990) 67

Second harmonic generation coefficients in push-pull polyenes: a model exact study, S. Ramasesha and P.K. Das 145 (1990) 343

Calculation of molecular *g* tensors. Comparison of Rayleigh-Schrödinger and Hartree-Fock perturbation theory, R. Angstl 145 (1990) 413

Molecular dynamics and scattering theory

Electronic structure of tert-butyl halides and group 14 derivatives: electron affinities and dissociative electron attachment, A. Modelli, F. Scagnolari, G. Distefano, M. Guerra and D. Jones 145 (1990) 89

A calculation of radiative lifetimes of electronically excited rovibronic levels of CuF, J. Schamps, J.M. Delaval and O. Faucher 145 (1990) 101

Non-empirical calculation of the Whitten-Rabinovitch coefficient, G. Song 145 (1990) 111

Model potential methods for the treatment of collisions between an excited rare gas and a ground state rare gas: accuracy and limitations, H. Kucal, D. Hennecart and F. Masnou-Seeuws 145 (1990) 163

A new look at the retention of orbital alignment in collisions involving atoms in ¹P electronic states: Ca(4s5p ¹P) + He, B. Pouilly and M.H. Alexander 145 (1990) 191

Experimental and theoretical studies of simple attractive Penning ionization systems, A. Merz, M.W. Müller, M.-W. Ruf, H. Hotop, W. Meyer and M. Movre 145 (1990) 219

The validity of the local approximation in Penning ionization as studied by model calculations, H. Morgner 145 (1990) 239

A close-coupling theory of associative detachment of electrons from negative ions, S.E. Haywood and J.B. Delos 145 (1990) 253

Excitation transfer collisions of metastable Ar*, Kr* and Xe* atoms with N₂(X, $v=0$): collision energy dependence of excitation cross sections and product vibrational distribution of N₂(C³Π_u, $v'=0,1,2,3$), E.J.D. Vredenbregt, W. Boom, R.J.F. van Gerwen and H.C.W. Beijerinck

145 (1990) 267

Experimental

Magnetic resonances

The main regularities of SNP formation in biradicals on the photolysis of cycloalkanones, I.V. Koptyug, E.G. Bagryanskaya, Yu.A. Grishin and R.Z. Sagdeev

145 (1990) 375

Calculation of molecular g tensors. Comparison of Rayleigh–Schrödinger and Hartree–Fock perturbation theory, R. Angstl

145 (1990) 413

Microwave spectroscopy

The reorientational motion of substituted benzenes in the crystalline state. Dielectric relaxation of orthodinitrotetramethylbenzene and orthodinitrotetrachlorobenzene, H.A. Kołodziej, T. Głowiąk, S. Sorriso, V. Caia and M. Braghetti

145 (1990) 355

Raman spectroscopy

Intramolecular vibrational distribution in IR multiphoton excited CF₃CH₂OH, A.L. Malinovsky and E.A. Ryabov

145 (1990) 389

Visible and UV spectroscopy

A calculation of radiative lifetimes of electronically excited rovibronic levels of CuF, J. Schamps, J.M. Delaval and O. Faucher

145 (1990) 101

Resonantly enhanced external heavy atom effect in organic glasses, P. Petelenz and J. Fünfschilling

145 (1990) 333

Absorption and magnetic circular dichroism spectra of the compressed copper(II) ion in K₂ZnF₄, M.J. Riley, L. Dubicki, G. Moran, E.R. Krausz and I. Yamada

145 (1990) 363

Photoelectron and Auger spectroscopy

Photoelectron spectroscopy of the freon molecules CF₃Cl, CF₂Cl₂ and CFCl₃ using synchrotron radiation from 41 to 160 eV, G. Cooper, W. Zhang, C.E. Brion and K.H. Tan

145 (1990) 117

The treatment of electron correlation in aperiodic systems. III. Application to polypeptides, C.-M. Liegener, A. Sutjianto and J. Ladik

145 (1990) 385

X-ray spectroscopy

Resonances in the silicon L core level cross sections of fluoromethylsilane compounds characterized by photoabsorption spectroscopy and MS-X α calculations, J.D. Bozek, G.M. Bancroft and K.H. Tan

145 (1990) 131

Electron impact spectroscopy

Electronic structure of tert-butyl halides and group 14 derivatives: electron affinities and dissociative electron attachment, A. Modelli, F. Scagnolari, G. Distefano, M. Guerra and D. Jones

145 (1990) 89

Laser methods

Polarization effects in metastable neon atom ($\text{Ne}^*(^3\text{P}_2)$) on ground state neon atom collision at thermal energy, J. Baudon, F. Perales, Ch. Miniatura, J. Robert, G. Vassilev, J. Reinhardt and H. Haberland 145 (1990) 153

Preparation of a pure intense beam of metastable helium by laser cooling, A. Aspect, N. Vansteenkiste, R. Kaiser, H. Haberland and M. Karrais 145 (1990) 307

Collimation of a rubidium beam below the Doppler limit, B. Sheehy, S.-Q. Shang, P. van der Straten and H. Metcalf 145 (1990) 317

A high intensity metastable neon trap, F. Shimizu, K. Shimizu and H. Takuma 145 (1990) 327

Synchrotron spectroscopies

Photoelectron spectroscopy of the freon molecules CF_3Cl , CF_2Cl_2 and CFCl_3 using synchrotron radiation from 41 to 160 eV, G. Cooper, W. Zhang, C.E. Brion and K.H. Tan 145 (1990) 117

Resonances in the silicon L core level cross sections of fluoromethylsilane compounds characterized by photoabsorption spectroscopy and MS-X α calculations, J.D. Bozek, G.M. Bancroft and K.H. Tan 145 (1990) 131

Coherent optical spectroscopy

Polarization effects in metastable neon atom ($\text{Ne}^*(^3\text{P}_2)$) on ground state neon atom collision at thermal energy, J. Baudon, F. Perales, Ch. Miniatura, J. Robert, G. Vassilev, J. Reinhardt and H. Haberland 145 (1990) 153

Optical pumping

Preparation of a pure intense beam of metastable helium by laser cooling, A. Aspect, N. Vansteenkiste, R. Kaiser, H. Haberland and M. Karrais 145 (1990) 307

Multiple resonance spectroscopy

The main regularities of SNP formation in biradicals on the photolysis of cycloalkanones, I.V. Koptyug, E.G. Bagryanskaya, Yu.A. Grishin and R.Z. Sagdeev 145 (1990) 375

Atomic and molecular beam techniques

Polarization effects in metastable neon atom ($\text{Ne}^*(^3\text{P}_2)$) on ground state neon atom collision at thermal energy, J. Baudon, F. Perales, Ch. Miniatura, J. Robert, G. Vassilev, J. Reinhardt and H. Haberland 145 (1990) 153

A crossed beam study of the ionization of molecules by metastable neon atoms, A. Aguilar, B. Brunetti, M. González and F. Vecchiocattivi 145 (1990) 211

Experimental and theoretical studies of simple attractive Penning ionization systems, A. Merz, M.W. Müller, M.-W. Ruf, H. Hotop, W. Meyer and M. Movre 145 (1990) 219

Excitation transfer collisions of metastable Ar^* , Kr^* and Xe^* atoms with $\text{N}_2(\text{X}, \nu=0)$: collision energy dependence of excitation cross sections and product vibrational distribution of $\text{N}_2(\text{C}^3\Pi_u, \nu'=0,1,2,3)$, E.J.D. Vredenbregt, W. Boom, R.J.F. van Gerwen and H.C.W. Beijerinck 145 (1990) 267

Scattering of magnetically analyzed $\text{F}(^2\text{P})$ atoms and their interactions with He , Ne , H_2 and CH_4 , V. Aquilanti, R. Candori, D. Cappelletti, E. Luzzatti and F. Pirani 145 (1990) 293

Preparation of a pure intense beam of metastable helium by laser cooling, A. Aspect, N. Vansteenkiste, R. Kaiser, H. Haberland and M. Karrais 145 (1990) 307

Collimation of a rubidium beam below the Doppler limit, B. Sheehy, S.-Q. Shang, P. van der Straten and H. Metcalf 145 (1990) 317

A high intensity metastable neon trap, F. Shimizu, K. Shimizu and H. Takuma 145 (1990) 327

Time-resolved experiments

A calculation of radiative lifetimes of electronically excited rovibronic levels of CuF,

J. Schamps, J.M. Delaval and O. Faucher

Resonantly enhanced external heavy atom effect in organic glasses, P. Petelenz and J. Fünfschilling

Intramolecular vibrational distribution in IR multiphoton excited $\text{CF}_3\text{CH}_2\text{OH}$, A.L. Malinovsky and E.A. Ryabov

145 (1990) 101

145 (1990) 333

145 (1990) 389

Measurement of macroscopic variables

Thermal conductivity of a moderately dense gas, C.A. Nieto de Castro, D.G. Friend, R.A. Perkins and J.C. Rainwater

145 (1990) 19

OBJECTS

Bulk systems

Gases

Thermal conductivity of a moderately dense gas, C.A. Nieto de Castro, D.G. Friend, R.A. Perkins and J.C. Rainwater

145 (1990) 19

Electronic structure of tert-butyl halides and group 14 derivatives: electron affinities and dissociative electron attachment, A. Modelli, F. Scagnolari, G. Distefano, M. Guerra and D. Jones

145 (1990) 89

Non-empirical calculation of the Whitten-Rabinovitch coefficient, G. Song

145 (1990) 111

Scattering of magnetically analyzed $\text{F}({}^2\text{P})$ atoms and their interactions with He, Ne, H_2 and CH_4 , V. Aquilanti, R. Candori, D. Cappelletti, E. Luzzatti and F. Pirani

145 (1990) 293

Intramolecular vibrational distribution in IR multiphoton excited $\text{CF}_3\text{CH}_2\text{OH}$, A.L. Malinovsky and E.A. Ryabov

145 (1990) 389

Supersonic beams

Preparation of a pure intense beam of metastable helium by laser cooling, A. Aspect, N. Vansteenkiste, R. Kaiser, H. Haberland and M. Karrais

145 (1990) 307

Liquid mixtures and solutions

The main regularities of SNP formation in biradicals on the photolysis of cycloalkanones,

I.V. Koptyug, E.G. Bagryanskaya, Yu.A. Grishin and R.Z. Sagdeev

145 (1990) 375

Crystals

The reorientational motion of substituted benzenes in the crystalline state. Dielectric relaxation of orthodinitrotetramethylbenzene and orthodinitrotetrachlorobenzene,

H.A. Kołodziej, T. Głowiąk, S. Sorriso, V. Caia and M. Braghetti

145 (1990) 355

Absorption and magnetic circular dichroism spectra of the compressed copper(II) ion in

K_2ZnF_4 , M.J. Riley, L. Dubicki, G. Moran, E.R. Krausz and I. Yamada

145 (1990) 363

-mixed

Absorption and magnetic circular dichroism spectra of the compressed copper(II) ion in

K_2ZnF_4 , M.J. Riley, L. Dubicki, G. Moran, E.R. Krausz and I. Yamada

145 (1990) 363

Glasses

Resonantly enhanced external heavy atom effect in organic glasses, P. Petelenz and J. Fünfschilling 145 (1990) 333

Polymers

Second harmonic generation coefficients in push-pull polyenes: a model exact study, S. Ramasesha and P.K. Das 145 (1990) 343

The treatment of electron correlation in aperiodic systems. III. Application to polypeptides, C.-M. Liegener, A. Sutjianto and J. Ladik 145 (1990) 385

Plasmas

A crossed beam study of the ionization of molecules by metastable neon atoms, A. Aguilar, B. Brunetti, M. González and F. Vecchiocattivi 145 (1990) 211

*Microscopic systems**Atoms*

Polarization effects in metastable neon atom ($\text{Ne}^*(^3\text{P}_2)$) on ground state neon atom collision at thermal energy, J. Baudon, F. Perales, Ch. Miniatura, J. Robert, G. Vassilev, J. Reinhardt and H. Haberland 145 (1990) 153

A new look at the retention of orbital alignment in collisions involving atoms in ^1P electronic states: $\text{Ca}(4s5p\,^1\text{P}) + \text{He}$, B. Pouilly and M.H. Alexander 145 (1990) 191

A close-coupling theory of associative detachment of electrons from negative ions, S.E. Haywood and J.B. Delos 145 (1990) 253

Scattering of magnetically analyzed $\text{F}(^2\text{P})$ atoms and their interactions with He, Ne, H_2 and CH_4 , V. Aquilanti, R. Candori, D. Cappelletti, E. Luzzatti and F. Pirani 145 (1990) 293

Preparation of a pure intense beam of metastable helium by laser cooling, A. Aspect, N. Vansteenkiste, R. Kaiser, H. Haberland and M. Karrais 145 (1990) 307

Collimation of a rubidium beam below the Doppler limit, B. Sheehy, S.-Q. Shang, P. van der Straten and H. Metcalf 145 (1990) 317

A high intensity metastable neon trap, F. Shimizu, K. Shimizu and H. Takuma 145 (1990) 327

Molecules (neutral and ionic)

Coordination structures and vibrational frequencies of Li and Na metaphosphates and nitrates. An ab initio SCF study, F. Ramondo, L. Bencivenni, R. Caminiti and F. Grandinetti 145 (1990) 27

Iterative methods to compute one- and two-dimensional Franck-Condon factors. Tests of accuracy and application to study indirect molecular transitions, J. Lermé 145 (1990) 67

Electronic structure of tert-butyl halides and group 14 derivatives: electron affinities and dissociative electron attachment, A. Modelli, F. Scagnolari, G. Distefano, M. Guerra and D. Jones 145 (1990) 89

-diatomic

A calculation of radiative lifetimes of electronically excited rovibronic levels of CuF , J. Schamps, J.M. Delaval and O. Faucher 145 (1990) 101

Model potential methods for the treatment of collisions between an excited rare gas and a ground state rare gas: accuracy and limitations, H. Kucal, D. Hennecart and F. Masnou-Seeuws 145 (1990) 163

Theoretical study of the electronic structure of the ArKr* exciplex, F. Spiegelmann, F.X. Gadea and M.C. Castex 145 (1990) 173

Experimental and theoretical studies of simple attractive Penning ionization systems, A. Merz, M.W. Müller, M.-W. Ruf, H. Hotop, W. Meyer and M. Movre 145 (1990) 219

-small polyatomics

Intramolecular and reactive dynamics of OH-overtone excited HOOH(D): a classical trajectory study on a quasiseparable potential surface, C. Getino, B.G. Sumpter and J. Santamaría 145 (1990) 1

Consistent force field modeling of matrix isolated molecules. V. Minimum energy path potential to the conformer conversion of 1,2-difluoroethane:Ar₃₆₄, ab initio calculation of electric multipole moments and electric polarization contribution to the conversion barrier, R. Gunde, T.-K. Ha and H.H. Günthard 145 (1990) 37

Iterative methods to compute one- and two-dimensional Franck-Condon factors. Tests of accuracy and application to study indirect molecular transitions, J. Lermé 145 (1990) 67

Non-empirical calculation of the Whitten-Rabinovitch coefficient, G. Song 145 (1990) 111

Photoelectron spectroscopy of the freon molecules CF₃Cl, CF₂Cl₂ and CFCI₃ using synchrotron radiation from 41 to 160 eV, G. Cooper, W. Zhang, C.E. Brion and K.H. Tan 145 (1990) 117

Resonances in the silicon L core level cross sections of fluoromethylsilane compounds characterized by photoabsorption spectroscopy and MS-X α calculations, J.D. Bozek, G.M. Bancroft and K.H. Tan 145 (1990) 131

Intramolecular vibrational distribution in IR multiphoton excited CF₃CH₂OH, A.L. Malinovsky and E.A. Ryabov 145 (1990) 389

A systematic study of molecular vibrational anharmonicity and vibration-rotation interaction by self-consistent-field higher-derivative methods. Linear polyatomic molecules, W.D. Allen, Y. Yamaguchi, A.G. Császár, D.A. Clabo Jr., R.B. Remington and H.F. Schaefer III 145 (1990) 427

-aromatics

Calculation of molecular g tensors. Comparison of Rayleigh-Schrödinger and Hartree-Fock perturbation theory, R. Angstl 145 (1990) 413

-polymeric and biological

Second harmonic generation coefficients in push-pull polyenes: a model exact study, S. Ramasesha and P.K. Das 145 (1990) 343

Molecular aggregates

-van der Waals molecules

Scattering of magnetically analyzed F(²P) atoms and their interactions with He, Ne, H₂ and CH₄, V. Aquilanti, R. Candori, D. Cappelletti, E. Luzzatti and F. Pirani 145 (1990) 293

-clusters

Consistent force field modeling of matrix isolated molecules. V. Minimum energy path potential to the conformer conversion of 1,2-difluoroethane: Ar_{364} , ab initio calculation of electric multipole moments and electric polarization contribution to the conversion barrier, R. Gunde, T.-K. Ha and H.H. Günthard

145 (1990) 37

Free radicals (including hydronium and muonium)

The main regularities of SNP formation in biradicals on the photolysis of cycloalkanones, I.V. Koptyug, E.G. Bagryanskaya, Yu.A. Grishin and R.Z. Sagdeev

Spin symmetry and interaction mechanisms in free radical reactions, Y.-N. Chiu and M. Gong

145 (1990) 375

145 (1990) 397

Ions and charge carriers

A close-coupling theory of associative detachment of electrons from negative ions, S.E. Haywood and J.B. Delos

145 (1990) 253

PHENOMENA*Molecular structure*

Coordination structures and vibrational frequencies of Li and Na metaphosphates and nitrates. An ab initio SCF study, F. Ramondo, L. Bencivenni, R. Caminiti and F. Grandinetti

145 (1990) 27

The reorientational motion of substituted benzenes in the crystalline state. Dielectric relaxation of orthodinitrotetramethylbenzene and orthodinitrotetrachlorobenzene, H.A. Kołodziej, T. Głowiak, S. Sorriso, V. Caia and M. Braghetti

145 (1990) 355

A systematic study of molecular vibrational anharmonicity and vibration-rotation interaction by self-consistent-field higher-derivative methods. Linear polyatomic molecules, W.D. Allen, Y. Yamaguchi, A.G. Császár, D.A. Clabo Jr., R.B. Remington and H.F. Schaefer III

145 (1990) 427

Vibrations and rotations of molecules

Intramolecular and reactive dynamics of OH-overtone excited $\text{HOOH}(\text{D})$: a classical trajectory study on a quasiseparable potential surface, C. Getino, B.G. Sumpter and J. Santamaría

145 (1990) 1

A systematic study of molecular vibrational anharmonicity and vibration-rotation interaction by self-consistent-field higher-derivative methods. Linear polyatomic molecules, W.D. Allen, Y. Yamaguchi, A.G. Császár, D.A. Clabo Jr., R.B. Remington and H.F. Schaefer III

145 (1990) 427

Electronic structure and states

Electronic structure of tert-butyl halides and group 14 derivatives: electron affinities and dissociative electron attachment, A. Modelli, F. Scagnolari, G. Distefano, M. Guerra and D. Jones

145 (1990) 89

Photoelectron spectroscopy of the freon molecules CF_3Cl , CF_2Cl_2 and CFCl_3 using synchrotron radiation from 41 to 160 eV, G. Cooper, W. Zhang, C.E. Brion and K.H. Tan

145 (1990) 117

Resonances in the silicon L core level cross sections of fluoromethylsilane compounds characterized by photoabsorption spectroscopy and MS-X α calculations, J.D. Bozek, G.M. Bancroft and K.H. Tan

145 (1990) 131

Theoretical study of the electronic structure of the ArKr* exciplex, F. Spiegelmann, F.X. Gadea and M.C. Castex 145 (1990) 173

Experimental and theoretical studies of simple attractive Penning ionization systems, A. Merz, M.W. Müller, M.-W. Ruf, H. Hotop, W. Meyer and M. Movre 145 (1990) 219

Second harmonic generation coefficients in push-pull polyenes: a model exact study, S. Ramasesha and P.K. Das 145 (1990) 343

Absorption and magnetic circular dichroism spectra of the compressed copper(II) ion in K_2ZnF_4 , M.J. Riley, L. Dubicki, G. Moran, E.R. Krausz and I. Yamada 145 (1990) 363

Electric and magnetic properties

Consistent force field modeling of matrix isolated molecules. V. Minimum energy path potential to the conformer conversion of 1,2-difluoroethane: Ar_{364} , ab initio calculation of electric multipole moments and electric polarization contribution to the conversion barrier, R. Gunde, T.-K. Ha and H.H. Günthard 145 (1990) 37

Calculation of molecular *g* tensors. Comparison of Rayleigh-Schrödinger and Hartree-Fock perturbation theory, R. Angstl 145 (1990) 413

Molecular interactions

Polarization effects in metastable neon atom ($Ne^*(^3P_2)$) on ground state neon atom collision at thermal energy, J. Baudon, F. Perales, Ch. Miniatura, J. Robert, G. Vassilev, J. Reinhardt and H. Haberland 145 (1990) 153

Model potential methods for the treatment of collisions between an excited rare gas and a ground state rare gas: accuracy and limitations, H. Kucal, D. Hennecart and F. Masnou-Seeuws 145 (1990) 163

Experimental and theoretical studies of simple attractive Penning ionization systems, A. Merz, M.W. Müller, M.-W. Ruf, H. Hotop, W. Meyer and M. Movre 145 (1990) 219

Excitation transfer collisions of metastable Ar*, Kr* and Xe* atoms with $N_2(X, v=0)$: collision energy dependence of excitation cross sections and product vibrational distribution of $N_2(C^3\Pi_u, v'=0,1,2,3)$, E.J.D. Vredenbregt, W. Boom, R.J.F. van Gerwen and H.C.W. Beijerinck 145 (1990) 267

Scattering of magnetically analyzed $F(^2P)$ atoms and their interactions with He, Ne, H_2 and CH_4 , V. Aquilanti, R. Candori, D. Cappelletti, E. Luzzatti and F. Pirani 145 (1990) 293

Spin symmetry and interaction mechanisms in free radical reactions, Y.-N. Chiu and M. Gong 145 (1990) 397

Spectral bandshapes and intensities

A calculation of radiative lifetimes of electronically excited rovibronic levels of CuF, J. Schamps, J.M. Delaval and O. Faucher 145 (1990) 101

Absorption and magnetic circular dichroism spectra of the compressed copper(II) ion in K_2ZnF_4 , M.J. Riley, L. Dubicki, G. Moran, E.R. Krausz and I. Yamada 145 (1990) 363

Coupling of electronic and nuclear motion

A calculation of radiative lifetimes of electronically excited rovibronic levels of CuF, J. Schamps, J.M. Delaval and O. Faucher 145 (1990) 101

Polarization effects in metastable neon atom ($Ne^*(^3P_2)$) on ground state neon atom collision at thermal energy, J. Baudon, F. Perales, Ch. Miniatura, J. Robert, G. Vassilev, J. Reinhardt and H. Haberland 145 (1990) 153

Energy transfer processes

Model potential methods for the treatment of collisions between an excited rare gas and a ground state rare gas: accuracy and limitations, H. Kucal, D. Hennecart and F. Masnou-Seeuws 145 (1990) 163

A new look at the retention of orbital alignment in collisions involving atoms in 1P electronic states: $\text{Ca}(4s5p\,{}^1P) + \text{He}$, B. Pouilly and M.H. Alexander 145 (1990) 191

Excitation transfer collisions of metastable Ar^* , Kr^* and Xe^* atoms with $\text{N}_2(\text{X}, \nu=0)$: collision energy dependence of excitation cross sections and product vibrational distribution of $\text{N}_2(\text{C}^3\Pi_u, \nu'=0,1,2,3)$, E.J.D. Vredenbregt, W. Boom, R.J.F. van Gerwen and H.C.W. Beijerinck 145 (1990) 267

Resonantly enhanced external heavy atom effect in organic glasses, P. Petelenz and J. Fünfschilling 145 (1990) 333

Molecular photophysical processes

Photoelectron spectroscopy of the freon molecules CF_3Cl , CF_2Cl_2 and CFCl_3 using synchrotron radiation from 41 to 160 eV, G. Cooper, W. Zhang, C.E. Brion and K.H. Tan 145 (1990) 117

Intramolecular dynamics

Intramolecular and reactive dynamics of OH-overtone excited $\text{HOOH}(\text{D})$: a classical trajectory study on a quasiseparable potential surface, C. Getino, B.G. Sumpter and J. Santamaria 145 (1990) 1

Consistent force field modeling of matrix isolated molecules. V. Minimum energy path potential to the conformer conversion of 1,2-difluoroethane: Ar_{364} , ab initio calculation of electric multipole moments and electric polarization contribution to the conversion barrier, R. Gunde, T.-K. Ha and H.H. Günthard 145 (1990) 37

-vibrational energy redistribution (including vibrational dissociation)

Intramolecular vibrational distribution in IR multiphoton excited $\text{CF}_3\text{CH}_2\text{OH}$, A.L. Malinovsky and E.A. Ryabov 145 (1990) 389

Luminescence spectra, yields and lifetimes

Resonantly enhanced external heavy atom effect in organic glasses, P. Petelenz and J. Fünfschilling 145 (1990) 333

Multiphoton phenomena

Intramolecular vibrational distribution in IR multiphoton excited $\text{CF}_3\text{CH}_2\text{OH}$, A.L. Malinovsky and E.A. Ryabov 145 (1990) 389

Reactions (including dissociation)

Intramolecular and reactive dynamics of OH-overtone excited $\text{HOOH}(\text{D})$: a classical trajectory study on a quasiseparable potential surface, C. Getino, B.G. Sumpter and J. Santamaria 145 (1990) 1

A close-coupling theory of associative detachment of electrons from negative ions, S.E. Haywood and J.B. Delos 145 (1990) 253

Spin symmetry and interaction mechanisms in free radical reactions, Y.-N. Chiu and M. Gong 145 (1990) 397

-gas phase

Non-empirical calculation of the Whitten-Rabinovitch coefficient, G. Song 145 (1990) 111

-photochemical

Second harmonic generation coefficients in push-pull polyenes: a model exact study, S. Ramasesha and P.K. Das 145 (1990) 343

The main regularities of SNP formation in biradicals on the photolysis of cycloalkanones, I.V. Koptyug, E.G. Bagryanskaya, Yu.A. Grishin and R.Z. Sagdeev 145 (1990) 375

Spin symmetry and interaction mechanisms in free radical reactions, Y.-N. Chiu and M. Gong 145 (1990) 397

Ionization (including Rydberg states)

A crossed beam study of the ionization of molecules by metastable neon atoms, A. Aguilar, B. Brunetti, M. González and F. Vecchiocattivi 145 (1990) 211

Experimental and theoretical studies of simple attractive Penning ionization systems, A. Merz, M.W. Müller, M.-W. Ruf, H. Hotop, W. Meyer and M. Movre 145 (1990) 219

A close-coupling theory of associative detachment of electrons from negative ions, S.E. Haywood and J.B. Delos 145 (1990) 253

Molecular motion (including diffusive)

Collimation of a rubidium beam below the Doppler limit, B. Sheehy, S.-Q. Shang, P. van der Straten and H. Metcalf 145 (1990) 317

A high intensity metastable neon trap, F. Shimizu, K. Shimizu and H. Takuma 145 (1990) 327

The reorientational motion of substituted benzenes in the crystalline state. Dielectric relaxation of orthodinitrotetramethylbenzene and orthodinitrotetrachlorobenzene, H.A. Kołodziej, T. Głowiąk, S. Sorriso, V. Caia and M. Braghetta 145 (1990) 355

Thermodynamic and transport properties

Thermal conductivity of a moderately dense gas, C.A. Nieto de Castro, D.G. Friend, R.A. Perkins and J.C. Rainwater 145 (1990) 19

Phase transitions

The reorientational motion of substituted benzenes in the crystalline state. Dielectric relaxation of orthodinitrotetramethylbenzene and orthodinitrotetrachlorobenzene, H.A. Kołodziej, T. Głowiąk, S. Sorriso, V. Caia and M. Braghetta 145 (1990) 355

